

## The crystal structure of deerite

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### Abstract

The crystal structure of deerite [ $P2_1/a$ ,  $a = 10.786(8)$ ,  $b = 18.88(2)$ ,  $c = 9.564(9)$ Å,  $\beta = 107.45(5)^\circ$ ] from Panoche, California, has been investigated using intensity data collected with  $\text{MoK}\alpha$  radiation on a Picker FACS 1 diffractometer. The structure of the pseudocell with  $c' = c/3$  and space group  $P2_1/a$  has been determined and refined to a weighted residual index of 0.07. The pseudocell structure has disordered Si and oxygen positions, and there are only three possible ordered arrangements of these: the preferred full structure of deerite has a weighted residual index of 0.08, but it was not possible to refine it. The ideal structural formula is  $\text{Fe}_8^{2+}\text{Fe}_3^{3+}\text{O}_3[\text{Si}_6\text{O}_{17}](\text{OH})_5$ ,  $Z = 4$ . The structure is formed of two structural units continuous along the  $c$ -axis direction: (1) a strip of edge-sharing  $M$ -atom octahedra, six octahedra in width, oriented parallel to  $\{110\}$ , and (2) a hybrid single-double  $[\text{Si}_6\text{O}_{17}]$  silicate chain. Apical and lateral oxygens of the silicate chain are shared with  $M$  octahedra, but the familiar sandwich of tetrahedral-octahedral-tetrahedral coordination polyhedra is not well developed. The basal tetrahedral oxygens enclose a structural void.  $\text{Fe}^{3+}$  probably occupies the lateral sites in the octahedral strip.

Similar structural units have been reported recently for howieite, which is associated with deerite in rocks of the Franciscan Formation. The arrangement of the silicate chain in chain-silicate structures is constrained by the close-packed oxygen distances in the octahedral strip. This constraint results in a distinctly different structural topology in deerite and howieite compared to pyroxene and amphibole and imparts a characteristic distortion to the silicate chain. In particular, the sides of the six-membered rings in both deerite and howieite are buckled inward.

### Introduction

Deerite (along with howieite and zussmanite) occurs in blocks of riebeckite-stilpnomelane schists within metasediments of the Franciscan Formation, California. The type locality is the Laytonville quarry, Mendocino County (Agrell *et al.*, 1965). Deerite has also been reported in stilpnomelane schists, associated with glaucophane schists, in the French and Italian Alps (for example, Agrell and Gay, 1970).

Deerite is a hydrous ferrous, ferric silicate: the proposed formula for a half unit-cell content with  $(\text{O},\text{OH}) = 50$  is  $(\text{Mg}_{0.08}\text{Mn}_{0.86}\text{Fe}_{10.90}^{2+})_{11.84}(\text{Fe}_{3.89}^{3+}\text{Al}_{0.38})_{6.27}\text{Si}_{11.86}\text{O}_{39.95}(\text{OH})_{10.05}$  (Agrell *et al.*, 1967, footnote by Agrell). Agrell *et al.* (1965) report that it is monoclinic, space group  $P2_1/a$ , with  $a = 10.755(2)$ ,  $b = 18.870(6)$ ,  $c = 9.568(2)$ Å,  $\beta = 107.12(4)^\circ$ , density  $3.837 \text{ gm cm}^{-3}$ . It forms black acicular crystals, elongated parallel to  $c$  and lozenge-shaped in cross sec-

tion, with a good  $\{110\}$  cleavage. The crystals are twinned submicroscopically: the twin axis is  $[001]$ . More recently, Wenk (1974) has suggested that deerite is in fact orthorhombic, space group  $Pnma$ , with  $a = 18.885$ ,  $b = 3.182$  (needle axis),  $c = 10.337$ Å.

Characteristic Mössbauer spectra and magnetic susceptibility data for deerite have been reported by several laboratories, and the initial interpretations of these data resulted in a certain amount of controversy. Bancroft *et al.*, (1968) interpreted their room-temperature Mössbauer spectrum in terms of three quadrupole doublets:  $A, A'$ , assigned to  $\text{Fe}^{2+}$  in sixfold coordination;  $B, B'$ , assigned to  $\text{Fe}^{3+}$  in sixfold coordination;  $C, C'$ , assigned to  $\text{Fe}^{2+}$  in a distorted fourfold coordination. The fraction of the total Fe content of deerite accommodated in each of the sites, or group of sites, associated with these doublets is approximately 0.47, 0.37, and 0.16, respectively. In a subsequent Mössbauer study, Frank and Bunbury



Table 4. cont.

K	L	F <sub>O</sub>	F <sub>C</sub>	K	L	F <sub>O</sub>	F <sub>C</sub>	K	L	F <sub>O</sub>	F <sub>C</sub>	K	L	F <sub>O</sub>	F <sub>C</sub>	K	L	F <sub>O</sub>	F <sub>C</sub>
17	3	94	64		3	92	96		-6	239	230	5	0	170	159				
	-3	141	131	18	0	120	101	1	3	194	175	5	-3	89	75			H = 11	
18	0	180	188		-3	93	99		-3	74	75		-6	117	97				
19	0	113	98	19	-6	161	178	2	0	99	90	6	0	83	47	1	-6	145	111
	3	107	109						3	104	94		2	80	17	2	3	166	181
					H = 7				6	97	34		-6	162	153		-3	170	156
	H = 6								-3	241	227		-9	130	111		-4	78	5
				1	0	102	103		-6	290	285	7	0	280	262		-6	91	89
0	0	404	397		6	118	118	3	3	224	192		2	30	10	3	0	157	136
	3	245	265		-3	312	309		-3	196	185		3	108	79		3	103	102
	-3	113	106		-6	106	111		-6	217	213		-4	87	69		-6	155	133
	-5	79	36		-9	84	77	4	-3	112	84		-6	104	79	4	-3	170	149
	-9	81	85	2	0	165	151	5	0	154	135		-9	110	103		-9	117	86
1	-3	209	203		-3	368	350		3	175	170	8	-3	99	82	5	0	191	166
	-9	225	229	3	-6	231	230		-6	154	156		-6	125	130		-6	164	135
2	0	392	386	4	0	154	139	6	0	89	83	9	0	201	169		-7	90	3
	3	214	220		3	123	145		3	167	174		-3	113	98	6	-6	89	50
	-6	150	144		-2	68	23		6	142	139	10	0	251	213	7	1	78	13
	-9	111	75		-3	337	335		-6	127	134	11	0	156	153		-6	208	193
3	0	294	381	5	0	104	99	7	3	149	148		3	85	47	9	-3	93	52
	3	193	184		6	110	121		-6	105	93	12	-3	212	195		-6	131	121
	-3	116	119	6	0	194	165		-9	96	98	13	-3	127	120	10	-3	91	79
	-6	154	166		-3	209	200	8	0	273	284		-6	85	65		-6	206	193
4	3	85	90		-9	104	87		-6	243	235	14	-6	121	101		-7	88	1
	-4	87	104	7	6	167	191	9	0	203	191	15	-4	84	5	11	0	99	76
	-6	102	105		-3	183	176		3	131	121	16	-3	99	82		-6	145	126
5	0	268	259		-9	195	192	10	-3	157	140					12	-3	87	53
	-3	107	116	8	0	166	165		-6	127	117		H = 10			13	-3	121	102
	-10	82	14		3	83	90	11	3	141	140	0	0	187	193				
6	0	221	232		-3	92	68		-6	120	95		1	94	10		H = 12		
	-3	148	142	9	6	105	131	12	0	89	100		-9	118	123				
	-9	138	125		-6	87	82		-3	202	196	1	3	155	179	0	0	103	67
7	0	104	106	10	6	165	188	13	0	127	111		-3	193	183		-3	113	104
	-3	172	162		-5	74	20		-6	104	73	2	0	87	70		-6	110	121
	-9	195	208		-6	159	162	14	3	183	181		-9	136	126	1	0	116	98
8	0	289	266	11	0	80	34		-6	90	73	3	-3	216	191		-3	210	182
	6	142	194		6	100	123		-7	85	13	5	-3	189	173	2	0	140	133
	-3	127	123		-2	73	44	15	3	154	132		-6	89	81	3	-6	105	57
	-9	88	66		-3	98	98	16	-6	102	82		-7	87	9	5	0	109	73
9	3	101	108	12	3	174	188	18	-3	130	114	6	0	175	153	6	0	208	183
	6	86	119		-3	222	207						-3	187	178		-6	136	138
	-9	273	296		-6	143	153		H = 9				-6	108	76	7	0	114	91
10	0	183	169	13	0	96	113					7	-3	157	151				
	3	149	142		-3	117	123	1	0	142	137	8	-5	80	23		H = 13		
11	0	138	128	14	0	166	154		-9	167	165		-6	208	197				
	-6	247	265		-3	177	154	2	0	162	146	9	0	94	58	2	-3	209	178
12	3	181	188		-6	85	87		3	153	154		3	92	78	3	-3	151	110
	-6	118	108	15	-3	94	85		-3	140	109		-3	137	116		-6	149	117
13	-3	81	71		-7	98	10		-6	84	79		-6	120	116	6	-3	100	98
	-6	84	101	16	0	185	191		-9	199	187	11	0	146	130	6	-4	96	21
14	-3	206	208		3	91	74	3	0	202	190		2	86	12				
15	0	99	100	18	-6	184	152		-8	80	19		-3	108	137				
	-3	108	85					4	3	164	156	12	-6	85	86				
16	0	145	127		H = 8				-3	151	137	13	-6	146	95				
	-3	170	168						-6	93	106	14	-3	206	181				
17	0	117	127	0	-3	265	251		-9	194	183	15	-3	141	123				